Discretization Error Control for Constrained Aerodynamic Shape Optimization

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SIAM CSE 2019 Spokane, Washington, USA February 25, 2019

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2 Optimization Problem

3 Error Estimation and Mesh Adaptation

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5 Conclusions and Future Work

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How does discretization error affect optimization?

Design/Optimization: Numerical optimization + CFD analysis



Control the discretization error in the optimization!

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General optimization problem

• Determine the design variables **x** that minimize the objective function *J*^{adapt}:

 $\begin{array}{ll} \min_{\mathbf{x}} & J^{\mathrm{adapt}}(\mathbf{U},\mathbf{x}) \\ \mathrm{s.t.} & \mathbf{R}(\mathbf{U},\mathbf{x}) = \mathbf{0} \\ & \mathbf{R}^{\mathrm{trim}} = \mathbf{J}^{\mathrm{trim}} - \bar{\mathbf{J}}^{\mathrm{trim}} = \mathbf{0} \end{array}$

- Objective output J^{adapt}: directly targeted for mesh adaptation
- Trim outputs J^{trim}: indirectly affect the objective error
- $\bar{\mathbf{J}}^{trim}$: constant target values for trim outputs
- R(U, x): governing PDEs, e.g. flow equations
- Solve $R(\boldsymbol{U},\boldsymbol{x})$ to get the (flow) states solution \boldsymbol{U}

Optimality condition

Augmented Lagrangian function:

$$\mathcal{L}(\mathbf{U}, \mathbf{x}, \boldsymbol{\lambda}, \boldsymbol{\mu}) = J^{\text{adapt}}(\mathbf{U}, \mathbf{x}) + \boldsymbol{\lambda}^T \mathbf{R}(\mathbf{U}, \mathbf{x}) + \boldsymbol{\mu}^T \mathbf{R}^{\text{trim}}(\mathbf{U}, \mathbf{x})$$

First-order optimality (Karush-Kuhn-Tucker) condition:

$$\begin{split} \frac{\partial \mathcal{L}}{\partial x} &= \frac{\partial J^{adapt}}{\partial x} + \lambda^T \frac{\partial R}{\partial x} + \mu^T \frac{\partial R^{trim}}{\partial x} = 0 & \text{optimal design} \\ \frac{\partial \mathcal{L}}{\partial U} &= \frac{\partial J^{adapt}}{\partial U} + \lambda^T \frac{\partial R}{\partial U} + \mu^T \frac{\partial R^{trim}}{\partial U} = 0 & \text{coupled adjoint} \\ \frac{\partial \mathcal{L}}{\partial \lambda} &= R(U, x) = 0 & \text{physical feasibility} \\ \frac{\partial \mathcal{L}}{\partial \mu} &= R^{trim}(U, x) = 0 & \text{trim condition} \end{split}$$

Flow PDE solve, always physically feasible: $\frac{\partial \mathcal{L}}{\partial \lambda} = \mathbf{0}$ Choose coupled adjoint variables λ , such that, $\frac{\partial \mathcal{L}}{\partial U} = \mathbf{0}$

Coupled adjoints in constrained optimization

Coupled adjoints in constrained optimization:

$$\frac{\partial \mathcal{L}}{\partial \mathbf{U}} = \frac{\partial J^{\text{adapt}}}{\partial \mathbf{U}} + \boldsymbol{\lambda}^T \frac{\partial \mathbf{R}}{\partial \mathbf{U}} + \boldsymbol{\mu}^T \frac{\partial \mathbf{R}^{\text{trim}}}{\partial \mathbf{U}} = \mathbf{0}$$
$$\Rightarrow \boldsymbol{\lambda}^T = -\left(\frac{\partial J^{\text{adapt}}}{\partial \mathbf{U}} + \boldsymbol{\mu}^T \frac{\partial \mathbf{R}^{\text{trim}}}{\partial \mathbf{U}}\right) \frac{\partial \mathbf{R}}{\partial \mathbf{U}}^{-1} = (\boldsymbol{\Psi}^{\text{adapt}} + \boldsymbol{\Psi}^{\text{trim}} \boldsymbol{\mu})^T$$

Sensitivity analysis:

$$\begin{aligned} \frac{\partial \mathcal{L}}{\partial \mathbf{x}} &= \frac{\partial J^{\text{adapt}}}{\partial \mathbf{x}} + \mathbf{\lambda}^T \frac{\partial \mathbf{R}}{\partial \mathbf{x}} + \boldsymbol{\mu}^T \frac{\partial \mathbf{R}^{\text{trim}}}{\partial \mathbf{x}} \\ &= \frac{\partial J^{\text{adapt}}}{\partial \mathbf{x}} + (\mathbf{\Psi}^{\text{adapt}} + \mathbf{\Psi}^{\text{trim}} \boldsymbol{\mu})^T \frac{\partial \mathbf{R}}{\partial \mathbf{x}} + \boldsymbol{\mu}^T \frac{\partial \mathbf{J}^{\text{trim}}}{\partial \mathbf{x}} \\ &= \frac{\partial J^{\text{adapt}}}{\partial \mathbf{x}} + (\mathbf{\Psi}^{\text{adapt}})^T \frac{\partial \mathbf{R}}{\partial \mathbf{x}} + \boldsymbol{\mu}^T \left[\frac{\partial \mathbf{J}^{\text{trim}}}{\partial \mathbf{x}} + (\mathbf{\Psi}^{\text{trim}})^T \frac{\partial \mathbf{R}}{\partial \mathbf{x}} \right] \\ &= \frac{dJ^{\text{adapt}}}{d\mathbf{x}} + \boldsymbol{\mu}^T \frac{d\mathbf{J}^{\text{trim}}}{d\mathbf{x}} \end{aligned}$$

Reduced optimization problem

Full optimality condition:

$$\begin{split} \frac{\partial \mathcal{L}}{\partial \mathbf{x}} &= \frac{\partial J^{\text{adapt}}}{\partial \mathbf{x}} + \lambda^T \frac{\partial \mathbf{R}}{\partial \mathbf{x}} + \mu^T \frac{\partial \mathbf{R}^{\text{trim}}}{\partial \mathbf{x}} = \mathbf{0} & \text{optimal design} \\ \frac{\partial \mathcal{L}}{\partial \mathbf{U}} &= \frac{\partial J^{\text{adapt}}}{\partial \mathbf{U}} + \lambda^T \frac{\partial \mathbf{R}}{\partial \mathbf{U}} + \mu^T \frac{\partial \mathbf{R}^{\text{trim}}}{\partial \mathbf{U}} = \mathbf{0} & \text{coupled adjoint} \\ \frac{\partial \mathcal{L}}{\partial \lambda} &= \mathbf{R}(\mathbf{U}, \mathbf{x}) = \mathbf{0} & \text{physical feasibility} \\ \frac{\partial \mathcal{L}}{\partial \mu} &= \mathbf{R}^{\text{trim}}(\mathbf{U}, \mathbf{x}) = \mathbf{0} & \text{trim condition} \end{split}$$

Reduced optimization problem

Full optimality condition:

$$\begin{split} \frac{\partial \mathcal{L}}{\partial \mathbf{x}} &= \frac{\partial J^{\text{adapt}}}{\partial \mathbf{x}} + \lambda^T \frac{\partial \mathbf{R}}{\partial \mathbf{x}} + \mu^T \frac{\partial \mathbf{R}^{\text{trim}}}{\partial \mathbf{x}} = \mathbf{0} & \text{optimal design} \\ \frac{\partial \mathcal{L}}{\partial \mathbf{U}} &= \frac{\partial J^{\text{adapt}}}{\partial \mathbf{U}} + \lambda^T \frac{\partial \mathbf{R}}{\partial \mathbf{U}} + \mu^T \frac{\partial \mathbf{R}^{\text{trim}}}{\partial \mathbf{U}} = \mathbf{0} & \text{coupled adjoint} \\ \frac{\partial \mathcal{L}}{\partial \lambda} &= \mathbf{R}(\mathbf{U}, \mathbf{x}) = \mathbf{0} & \text{physical feasibility} \\ \frac{\partial \mathcal{L}}{\partial \mu} &= \mathbf{R}^{\text{trim}}(\mathbf{U}, \mathbf{x}) = \mathbf{0} & \text{trim condition} \end{split}$$

Reduced optimality condition (what the optimizer does):

$$\frac{\partial \mathcal{L}}{\partial \mathbf{x}} = \frac{dJ^{\text{adapt}}}{d\mathbf{x}} + \boldsymbol{\mu}^T \frac{d\mathbf{J}^{\text{trim}}}{d\mathbf{x}} = \mathbf{0}$$
$$\frac{\partial \mathcal{L}}{\partial \boldsymbol{\mu}} = \mathbf{R}^{\text{trim}} = \mathbf{0}$$

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Numerical error affects both objective and constraint outputs.

coarse space:
$$\mathbf{x}_0 \to \text{optimization} \to \underbrace{\mathbf{U}_H, \mathbf{x}_H^*}_{\text{optimal design}} \to J_H(\mathbf{U}_H, \mathbf{x}_H^*)$$

fine space: $\mathbf{x}_0 \to \text{optimization} \to \underbrace{\mathbf{U}_h, \mathbf{x}_h^*}_{\text{optimal design}} \to J_h(\mathbf{U}_h, \mathbf{x}_h^*)$

• Objective error estimates for the optimal design,

 $\delta J_{\text{opt}}^{\text{adapt}} = J_H^{\text{adapt}}(\mathbf{U}_H, \mathbf{x}_H^*) - J_h^{\text{adapt}}(\mathbf{U}_h, \mathbf{x}_h^*) = J_h^{\text{adapt}}(\mathbf{U}_h^H, \mathbf{x}_H^*) - J_h^{\text{adapt}}(\mathbf{U}_h, \mathbf{x}_h^*)$

Coarse space

 U_H

- State injection: $\mathbf{U}_h^H = \mathbf{I}_h^H \mathbf{U}_H$
- Fine space flow residual, $\mathbf{R}_h(\mathbf{U}_h^H, \mathbf{x}_H^*) \neq \mathbf{0}$
- Fine space trim residual, $\mathbf{R}_{h}^{\text{trim}}(\mathbf{U}_{h}^{H}, \mathbf{x}_{H}^{*}) = \mathbf{J}_{h}^{\text{trim}}(\mathbf{U}_{h}^{H}, \mathbf{x}_{H}^{*}) - \bar{\mathbf{J}}^{\text{trim}} = \mathbf{J}_{H}^{\text{trim}}(\mathbf{U}_{H}, \mathbf{x}_{H}^{*}) - \bar{\mathbf{J}}^{\text{trim}} = \mathbf{0}$



Fine space

injection: I_{k}^{H}

Recall the optimality condition:

$$\frac{\partial \mathcal{L}}{\partial \mathbf{U}} = \frac{\partial J^{\text{adapt}}}{\partial \mathbf{U}} + \lambda^T \frac{\partial \mathbf{R}}{\partial \mathbf{U}} + \mu^T \frac{\partial \mathbf{R}^{\text{trim}}}{\partial \mathbf{U}} = \mathbf{0}$$
$$\frac{\partial \mathcal{L}}{\partial \mathbf{x}} = \frac{\partial J^{\text{adapt}}}{\partial \mathbf{x}} + \lambda^T \frac{\partial \mathbf{R}}{\partial \mathbf{x}} + \mu^T \frac{\partial \mathbf{R}^{\text{trim}}}{\partial \mathbf{x}} = \mathbf{0}$$

Recall the optimality condition:



Recall the optimality condition:

$$\frac{\partial J^{\text{adapt}}}{\partial \mathbf{U}} = -\lambda^T \frac{\partial \mathbf{R}}{\partial \mathbf{U}} - \mu^T \frac{\partial \mathbf{R}^{\text{trim}}}{\partial \mathbf{U}}$$
$$\frac{\partial J^{\text{adapt}}}{\partial \mathbf{x}} = -\lambda^T \frac{\partial \mathbf{R}}{\partial \mathbf{x}} - \mu^T \frac{\partial \mathbf{R}^{\text{trim}}}{\partial \mathbf{x}}$$

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Error estimation using coupled adjoints

$$\delta J_{\text{opt}}^{\text{adapt}} = J_h^{\text{adapt}}(\mathbf{U}_h^H, \mathbf{x}_H^*) - J_h^{\text{adapt}}(\mathbf{U}_h, \mathbf{x}_h^*) = \frac{\partial J_h^{\text{adapt}}}{\partial \mathbf{U}_h} \delta \mathbf{U} + \frac{\partial J_h^{\text{adapt}}}{\partial \mathbf{x}} \delta \mathbf{x}$$
$$= -\lambda_h^T \frac{\partial \mathbf{R}_h}{\partial \mathbf{U}_h} \delta \mathbf{U} - \mu_h^T \frac{\partial \mathbf{R}_h^{\text{trim}}}{\partial \mathbf{U}_h} \delta \mathbf{U} - \lambda_h^T \frac{\partial \mathbf{R}_h}{\partial \mathbf{x}} \delta \mathbf{x} - \mu_h^T \frac{\partial \mathbf{R}_h^{\text{trim}}}{\partial \mathbf{x}} \delta \mathbf{x}$$
$$= -\lambda_h^T \left(\frac{\partial \mathbf{R}_h}{\partial \mathbf{U}_h} \delta \mathbf{U} + \frac{\partial \mathbf{R}_h}{\partial \mathbf{x}_h} \delta \mathbf{x} \right) - \mu_h \left(\frac{\partial \mathbf{R}_h^{\text{trim}}}{\partial \mathbf{U}_h} \delta \mathbf{U} + \frac{\partial \mathbf{R}_h^{\text{trim}}}{\partial \mathbf{x}_h} \delta \mathbf{x} \right)$$
$$= -\lambda_h^T \delta \mathbf{R}_h - \mu_h^T \delta \mathbf{R}_h^{\text{trim}}$$

Recall the optimality condition:

$$\frac{\partial J^{\text{adapt}}}{\partial \mathbf{U}} = -\boldsymbol{\lambda}^T \frac{\partial \mathbf{R}}{\partial \mathbf{U}} - \boldsymbol{\mu}^T \frac{\partial \mathbf{R}^{\text{trim}}}{\partial \mathbf{U}}$$
$$\frac{\partial J^{\text{adapt}}}{\partial \mathbf{x}} = -\boldsymbol{\lambda}^T \frac{\partial \mathbf{R}}{\partial \mathbf{x}} - \boldsymbol{\mu}^T \frac{\partial \mathbf{R}^{\text{trim}}}{\partial \mathbf{x}}$$

Error estimation using coupled adjoints

$$\begin{split} \delta J_{\text{opt}}^{\text{adapt}} &= J_h^{\text{adapt}}(\mathbf{U}_h^H, \mathbf{x}_H^*) - J_h^{\text{adapt}}(\mathbf{U}_h, \mathbf{x}_h^*) = \frac{\partial J_h^{\text{adapt}}}{\partial \mathbf{U}_h} \delta \mathbf{U} + \frac{\partial J_h^{\text{adapt}}}{\partial \mathbf{x}} \delta \mathbf{x} \\ &= -\lambda_h^T \frac{\partial \mathbf{R}_h}{\partial \mathbf{U}_h} \delta \mathbf{U} - \mu_h^T \frac{\partial \mathbf{R}_h^{\text{trim}}}{\partial \mathbf{U}_h} \delta \mathbf{U} - \lambda_h^T \frac{\partial \mathbf{R}_h}{\partial \mathbf{x}} \delta \mathbf{x} - \mu_h^T \frac{\partial \mathbf{R}_h^{\text{trim}}}{\partial \mathbf{x}} \delta \mathbf{x} \\ &= -\lambda_h^T \left(\frac{\partial \mathbf{R}_h}{\partial \mathbf{U}_h} \delta \mathbf{U} + \frac{\partial \mathbf{R}_h}{\partial \mathbf{x}_h} \delta \mathbf{x} \right) - \mu_h \left(\frac{\partial \mathbf{R}_h^{\text{trim}}}{\partial \mathbf{U}_h} \delta \mathbf{U} + \frac{\partial \mathbf{R}_h^{\text{trim}}}{\partial \mathbf{x}_h} \delta \mathbf{x} \right) \\ &= -\lambda_h^T \delta \mathbf{R}_h - \mu_h^T \delta \mathbf{R}_h^{\text{trim}} \\ &= -\lambda_h^T \mathbf{R}_h(\mathbf{U}_h^H, \mathbf{x}_H^*) \end{split}$$

Objective error estimates for the optimal design,

$$\delta J_{\text{opt}}^{\text{adapt}} = -\lambda_h^T \mathbf{R}_h(\mathbf{U}_h^H, \mathbf{x}_H^*)$$

= $-(\Psi_h^{\text{adapt}})^T \mathbf{R}_h(\mathbf{U}_h^H, \mathbf{x}_H^*) - \mu_h^T (\Psi_h^{\text{trim}})^T \mathbf{R}_h(\mathbf{U}_h^H, \mathbf{x}_H^*)$
= $\underbrace{\delta J^{\text{adapt}}(\mathbf{x}_H^*)}_{\text{objective error only}} + \underbrace{\mu_h^T \delta \mathbf{J}^{\text{trim}}(\mathbf{x}_H^*)}_{\text{inexact constraints satisfaction}}$

Error localization:

- Ψ_h : reconstruction using the coarse-space adjoints Ψ_H
- μ_h : extracted from the optimizer on the coarse space
- Adapt (error) indicator: $\eta_e = |\Psi_{h,e}^T \mathbf{R}_{h,e} (\mathbf{U}_h^H, \mathbf{x}_H)|$

• Combined indicator: $\eta_{e,\text{opt}} = \eta_e^{\text{adapt}} + |\boldsymbol{\mu}|^T \eta_e^{\text{trim}}$ Mesh adaptation:

- Hessian-based adaptation: refine mesh to control error
- Mesh optimization: optimize mesh (minimize error) given a fixed cost, $\mbox{cost} = \mbox{dim}(U)$

Adaptive multi-fidelity optimization

Error based multi-fidelity optimization: max allowable objective error $\downarrow \Rightarrow$ mesh refinement \Rightarrow fidelity \uparrow



Cost based multi-fidelity optimization:

given cost $\uparrow \Rightarrow$ mesh optimization \Rightarrow objective error $\downarrow \Rightarrow$ fidelity \uparrow



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1D advection diffusion problem

Governing equation

$$a\frac{\partial u}{\partial x} - \nu \frac{\partial^2 u}{\partial x^2} = 0, \quad x \in [0, L], \ u(0) = 0, \ u(L) = 1$$

where Peclet number can be defined as $Pe \equiv aL/\nu$ Analytic solution is given by

$$u(x) = \frac{\exp(Pe \times x/L) - 1}{\exp(Pe) - 1} \qquad \frac{\partial u}{\partial x} = \frac{Pe}{L} \frac{\exp(Pe \times x/L)}{\exp(Pe) - 1}$$

Optimization problem

$$\min_{\mathbf{x}=Pe} \quad J(\mathbf{x}) = -\frac{\partial u}{\partial x} \Big|_{x=0.76L}$$
s.t. $a \frac{\partial u}{\partial x} - \nu \frac{\partial^2 u}{\partial x^2} = 0$

Analytic solution: $\mathbf{x}^* = 3.8060$, $\mathcal{J}(\mathbf{x}^*) = -1.5615$

Optimization on different meshes (DG, p = 2, $N_e = 8$)



objective on different meshes

states solution *u* at spurious optima

Initial design	Mesh	$\ \mathbf{x}_{H}^{*}-\mathbf{x}^{*}\ $	$\ \delta J_H(\mathbf{x}_H^*)\ $	$\ J_H(\mathbf{x}_H^*) - \mathcal{J}(\mathbf{x}^*)\ $
$\mathbf{x}_0 = 40$	uniform	40.79686	0.15555	1.06446
	iso-adapted	0.08455	0.01309	0.01423
	optimized	0.00400	0.00063	0.00072
$x_0 = 20$	uniform	0.16022	0.02063	0.02109
	iso-adapted	0.03803	0.00505	0.00525
	optimized	0.00400	0.00063	0.00072

Inviscid transonic airfoil optimization



Inviscid transonic airfoil optimization



Optimization on different meshes (DG, p = 1, opt tol $= 1 \times 10^{-4}$)

	$C_{d,0}$	$c_{d,\text{opt}}$	$\delta c_{d,\mathrm{opt}}$	cost (dof)
Hessian-based Mesh optimization	2.242E-2	1.140E-3 1.136E-3	6.708E-5 8.752E-5	$\begin{array}{l} \sim 30000 \\ \sim 15000 \end{array}$

Why mesh optimization in shape optimization ?



optimized meshes (16th, 17th, 19th optimization step from left to right)

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Conclusions:

- Numerical error should be carefully controlled
- Traditional aerodynamic optimization a priori mesh, numerical error not controlled
- Error estimation + mesh adaptation actively controls the numerical error
- Prevent over-refining and over-optimizing during optimization

Future Work:

- Incorporate with sensitivity error estimates
- Accelerate error estimation and mesh adaptation process
- Combine with *h*-*p* refinement

Department of Energy DE-FG02-13ER26146/DE-SC0010341 Boeing Company, with technical monitor Dr. Mori Mani — Thank you —

Sensitivity verification









Airfoil parameterization

 Hicks-Henne basis functions: linear combination of "bump" functions added to the baseline airfoil



$$z = z_{\text{base}} + \sum_{i=0}^{n} a_i \phi_i(x)$$
$$\phi_i(x) = \sin^{t_i}(\pi x^{m_i})$$
$$m_i = \ln(0.5) / \ln(x_{M_i})$$

x: coord along the airfoil chordz: vertical surface coord x_{M_i} : maxima location t_i : width of the bump function

• Design parameters: $\mathbf{x} = [\alpha, a_1, a_2, \cdots, a_n]^T$ Coefficients of Hicks-Henne basis + angle of attack α

Mesh Movement

- Radial Basis Function (RBF): only depends on the distance from the origin or a center, e.g. $\phi(x) = e^{-x^2}$
- We can use a sum of RBFs φ(||x||) and a polynomial p(x) to interpolate the original function (mesh movement):

$$\vec{d}(\vec{x}) \approx \tilde{d}(\vec{x}) = \sum_{i=1}^{N_b} \vec{r}_i \phi(\|\vec{x} - \vec{x}_i\|) + \vec{p}(\vec{x})$$

- Solving for a linear system $\mathcal{O}(N_b)$ of $\vec{r_i}$
- Mesh connectivity information not required



Laminar airfoil optimization





Laminar low-speed airfoil optimization



initial design



optimized design (no adapt)



optimized design (adapt on drag)



optimized design (adapt on both)

Optimization on different meshes (DG, p = 1, opt tol = 1E-4)

	$\delta J^{ m adapt}$	$oldsymbol{\mu}_h^T \delta J^{ ext{trim}}$	$\delta J_{opt}^{\mathrm{adapt}}$	$\left\ \left(J_{h,p}^{\mathrm{adapt}} ight)^{*} - \left(J_{h,p+1}^{\mathrm{adapt}} ight)^{*} ight\ $
Fixed mesh	1.347E-4	1.456E-4	2.803E-4	2.013E-4
Adapt on drag	9.060E-5	8.490E-5	1.755E-4	1.758E-4
Adapt on both	8.402E-5	7.009E-6	9.103E-5	9.160E-5

Turbulent transonic airfoil optimization



Turbulent transonic airfoil optimization



Multi-point optimization



Multi-point optimization



Unstructured mesh adaptation and mesh optimization

Riemannian metric field $\mathcal{M} \in \mathbb{R}^{d \times d}$

Encode the discrete mesh (shape and size) with a continuous symmetric positive definite (SPD) tensor field, $\mathcal{M}(\vec{x}) \in \mathbb{R}^{d \times d}$

distance under the metric from \vec{x} to $\vec{x} + \delta \vec{x}$, $\delta l_{\mathcal{M}} = \sqrt{\delta \vec{x}^T \mathcal{M} \delta \vec{x}}$



- Eigenvectors ⇒ principle stretching direction
- Eigenvalues $\lambda_i = 1/h_i^2 \Rightarrow$ stretching magnitude

Unstructured mesh adaptation and mesh optimization

Metric conforming mesh

A mesh in which each edge has the same length under the metric



Anisotropic metric:

 \mathcal{M}_l

Mesh adaptation and mesh optimization techniques

- Hessian-based adaptation: refine mesh to control error solution Hessian $\frac{\partial^2 u}{\partial x_i \partial x_j} \Rightarrow$ eigenvectors \Rightarrow element shape error estimates $\eta_{e,opt} \Rightarrow$ eigenvalues magnitue \Rightarrow mesh size
- Mesh optimization: optimize mesh given a fixed cost Cost: $\dim(\mathbf{U}) \Rightarrow$ degrees of freedom (dof)

$$\min_{\mathcal{M}(\vec{x})} \sum \eta_{e,\text{opt}} \quad \text{s.t. } \cos t = \text{const}$$